Message

From: McCord, James [mccord.james@epa.gov]
Sent: 11/21/2017 7:13:32 PM
To: Buckley, Timothy [Buckley.Timothy@epa.gov]
CC: Strynar, Mark [Strynar.Mark@epa.gov]
Subject: RE: Sweeney Water NTA Assignments and Report
Attachments: reduced PFAS hits from Chemours Time Course.xlsx

Actually some of the formatting changes are in this version.
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James McCord

From: McCord, James
Sent: Tuesday, November 21, 2017 2:12 PM
To: Buckley, Timothy <Buckley.Timothy@epa.gov>
Cc: Mark Strynar (strynar.mark@epa.gov) <strynar.mark@epa.gov>
Subject: Sweeney Water NTA Assignments and Report

Hello Tim,

Mark and I went through an manually curated the list of extracted features from just the Sweeney Drinking water and compiled a spreadsheet with some assignments. I included the raw abundance values for each week for both Sweeney and Chemours outfall for comparison. Matches against the Richards list are highlighted in green. A few key points.

- The majority of the features from the initial search are not fluorinated, are fragments, adducts or dimers related to the known chemical species, or do not persist into the Sweeney drinking water from the outfall upon close inspection and have been removed. The result is 34 unique formulas assignments, three of which show two major isomers.
- The Richards compounds account for 21/36 (60%) of the remaining chemical features and 66% of the total signal abundance of fluorinated features.
- Compounds have a red label if they were reported to DEQ. Between the legacy PFAs and the nontargeted compounds already discussed this accounts for 65% of the total signal.
- Compound with a yellow label cannot be identified without our current setup because they either coelute with other compounds or are too low abundance to do reasonable feature assignment.
- There are 5 PFESA compounds we have identified that have not been reported on in the NTA work so far, the abundance of these varies drastically over time, as we discussed with the Nafion byproducts, and only the compounds 297.9548@5.09 and 365.9413@8.0889 have abundances at levels comparable to the reported species in the Sweeney water over the timescale sampled here.
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As a personal comment, the matching of the compounds against the list is good confirmation of a formula match, but our initial work with the triple quad leads me to suspect the structures in the water are different than those on the list even though they share a chemical formula. This is just a difference in positioning of the ether and fluoro- groups within the backbone which is yielding different fragmentation.

We would be happy to talk about any of these results if you want further clarification.
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James McCord